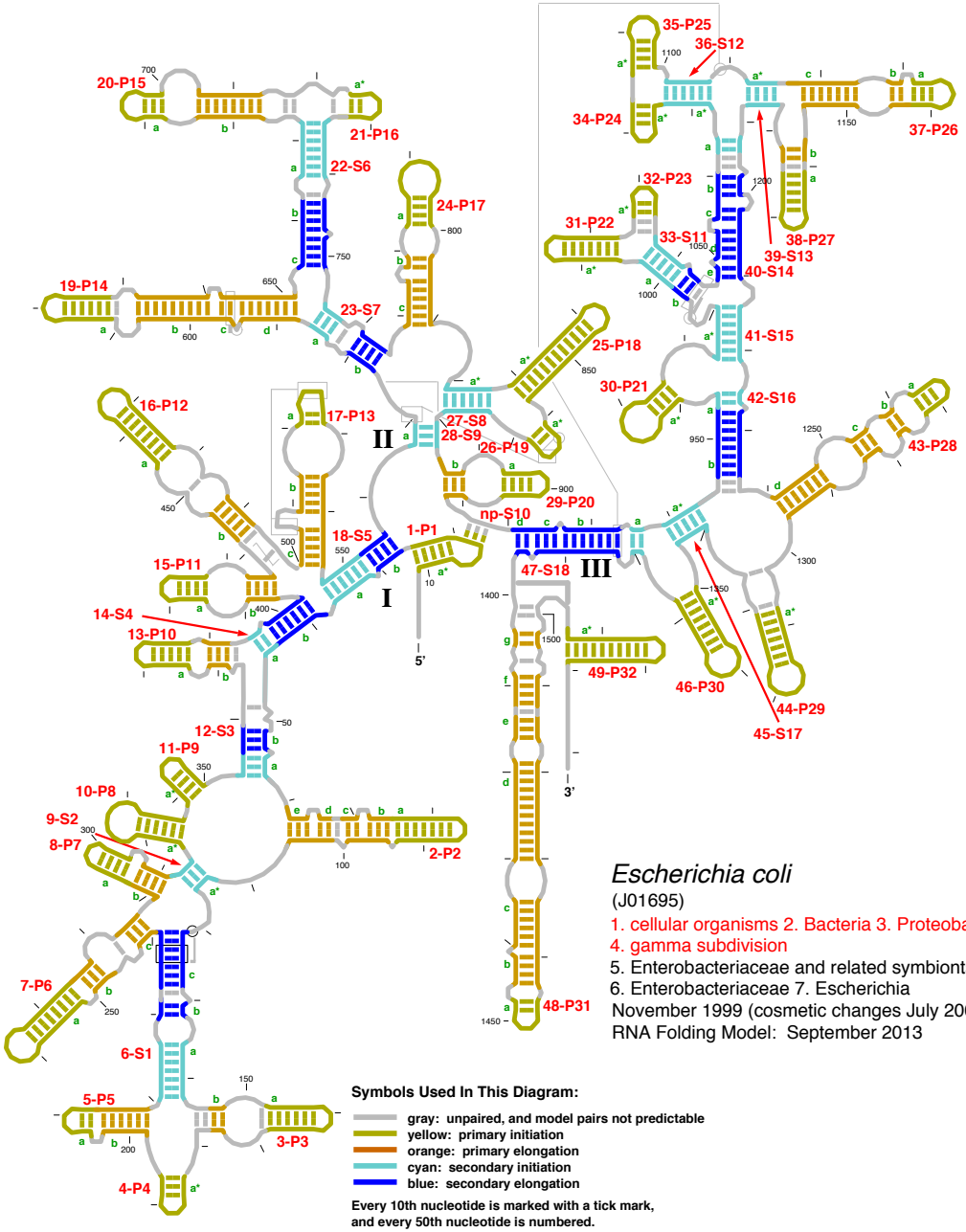
RNA CG Model Energy Profile

Ren Lab Meeting

01/24/14

Secondary Structure: small subunit ribosomal RNA



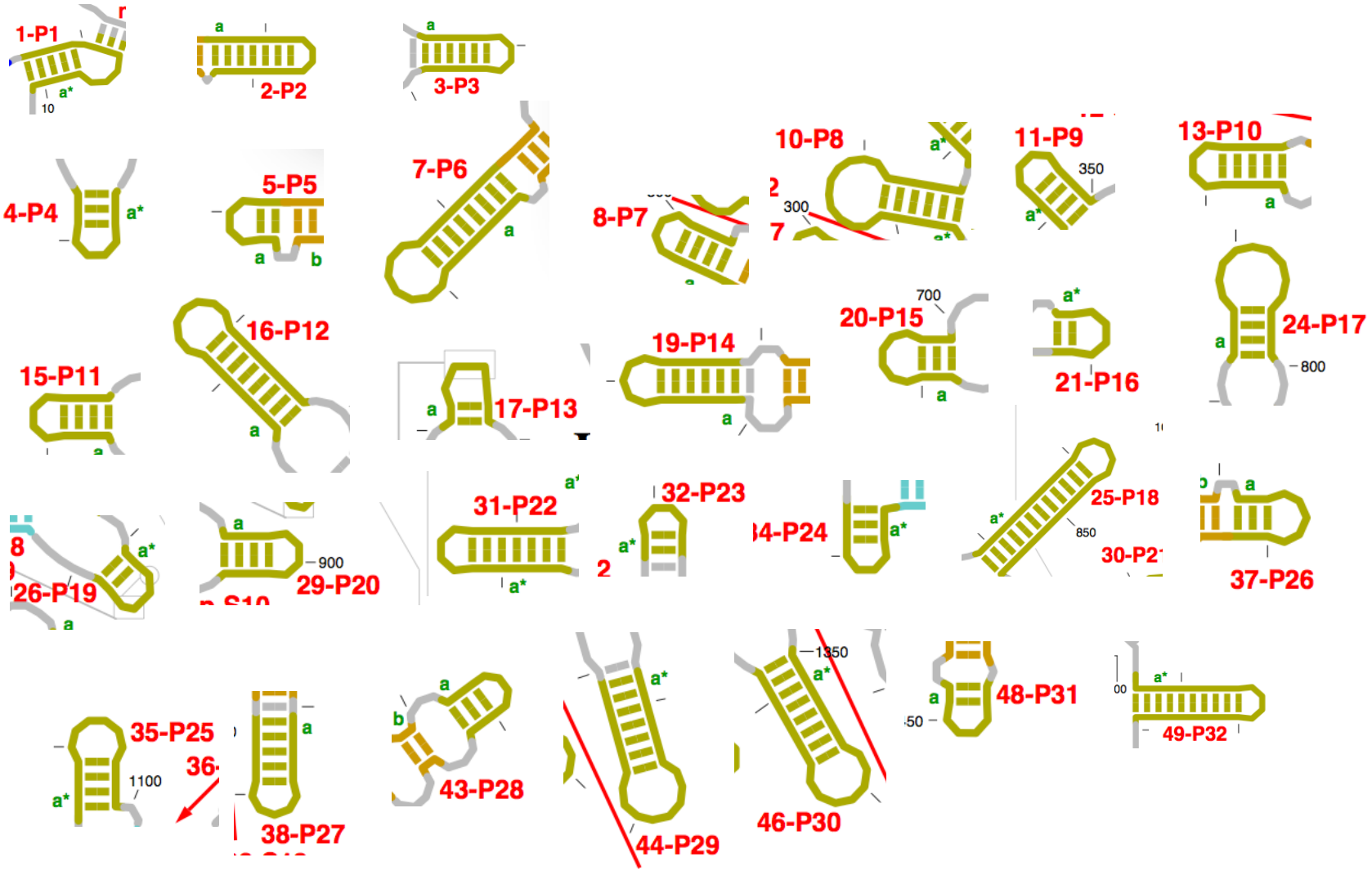
Escherichia coli
(J01695)
1. cellular organisms 2. Bacteria 3. Proteobacteria
4. gamma subdivision
5. Enterobacteriaceae and related symbionts
6. Enterobacteriaceae 7. Escherichia
November 1999 (cosmetic changes July 2001)
RNA Folding Model: September 2013

Symbols Used In This Diagram:

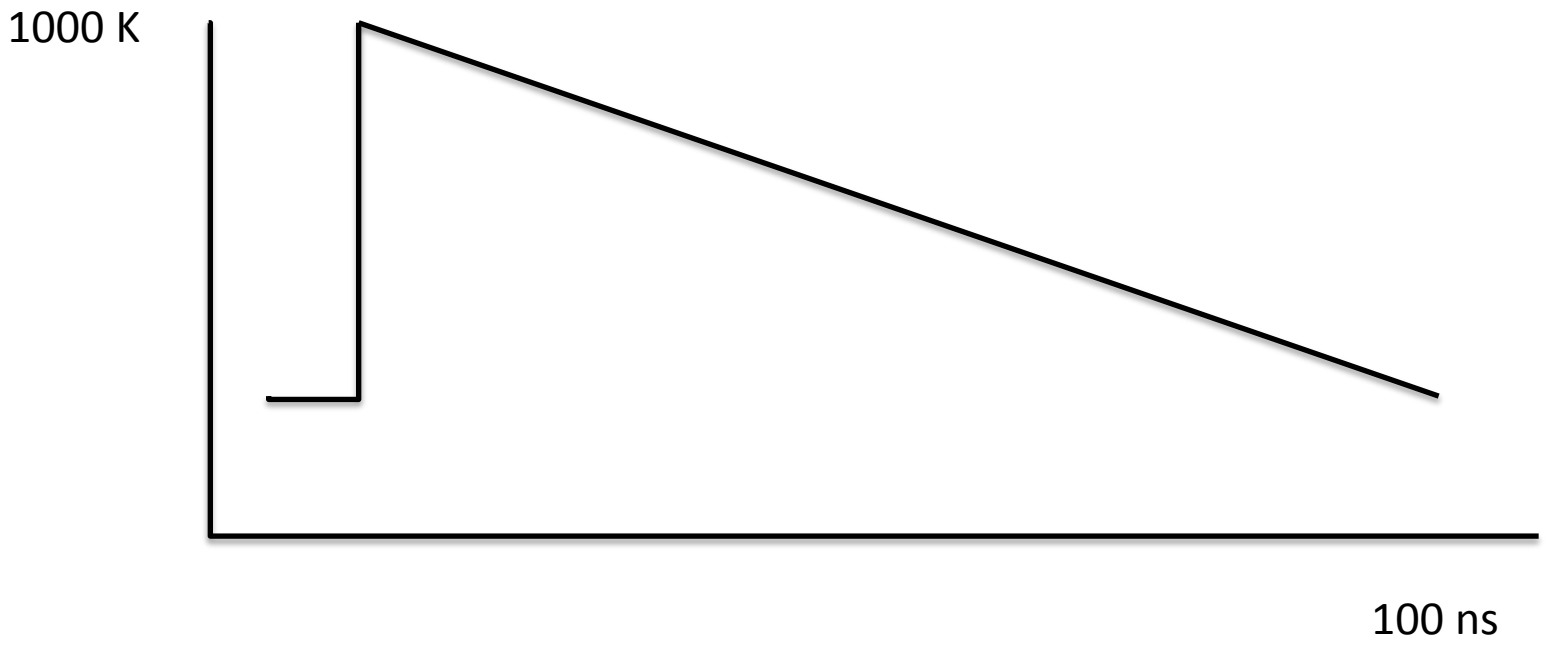
- gray: unpaired, and model pairs not predictable
- yellow: primary initiation
- orange: primary elongation
- cyan: secondary initiation
- blue: secondary elongation

Every 10th nucleotide is marked with a tick mark,
and every 50th nucleotide is numbered.

Hairpin Helices



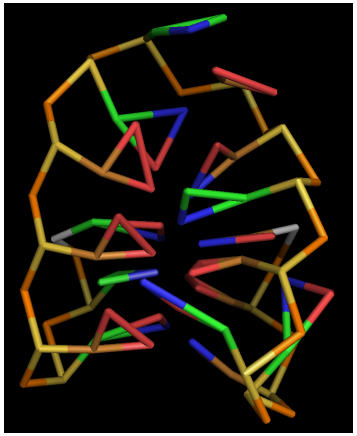
Simulated Annealing



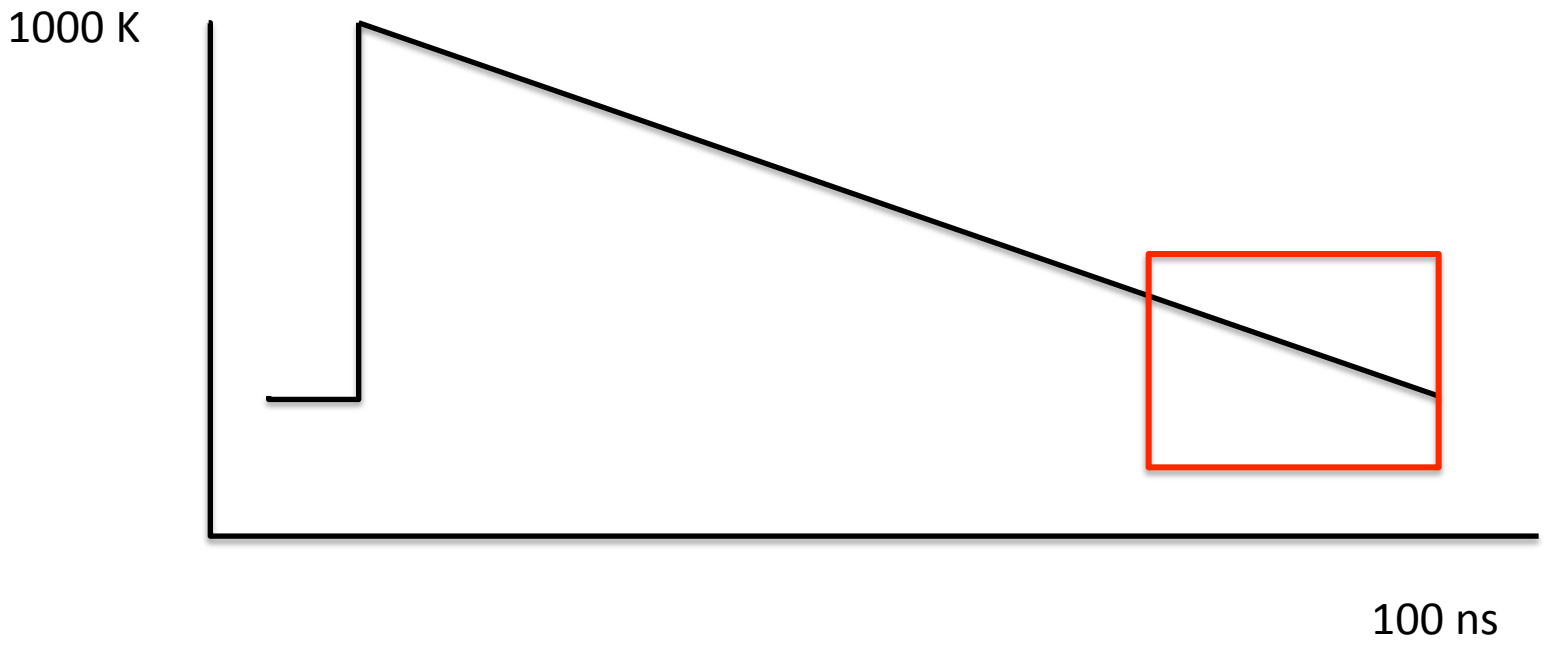


Linear Molecules





Simulated Annealing



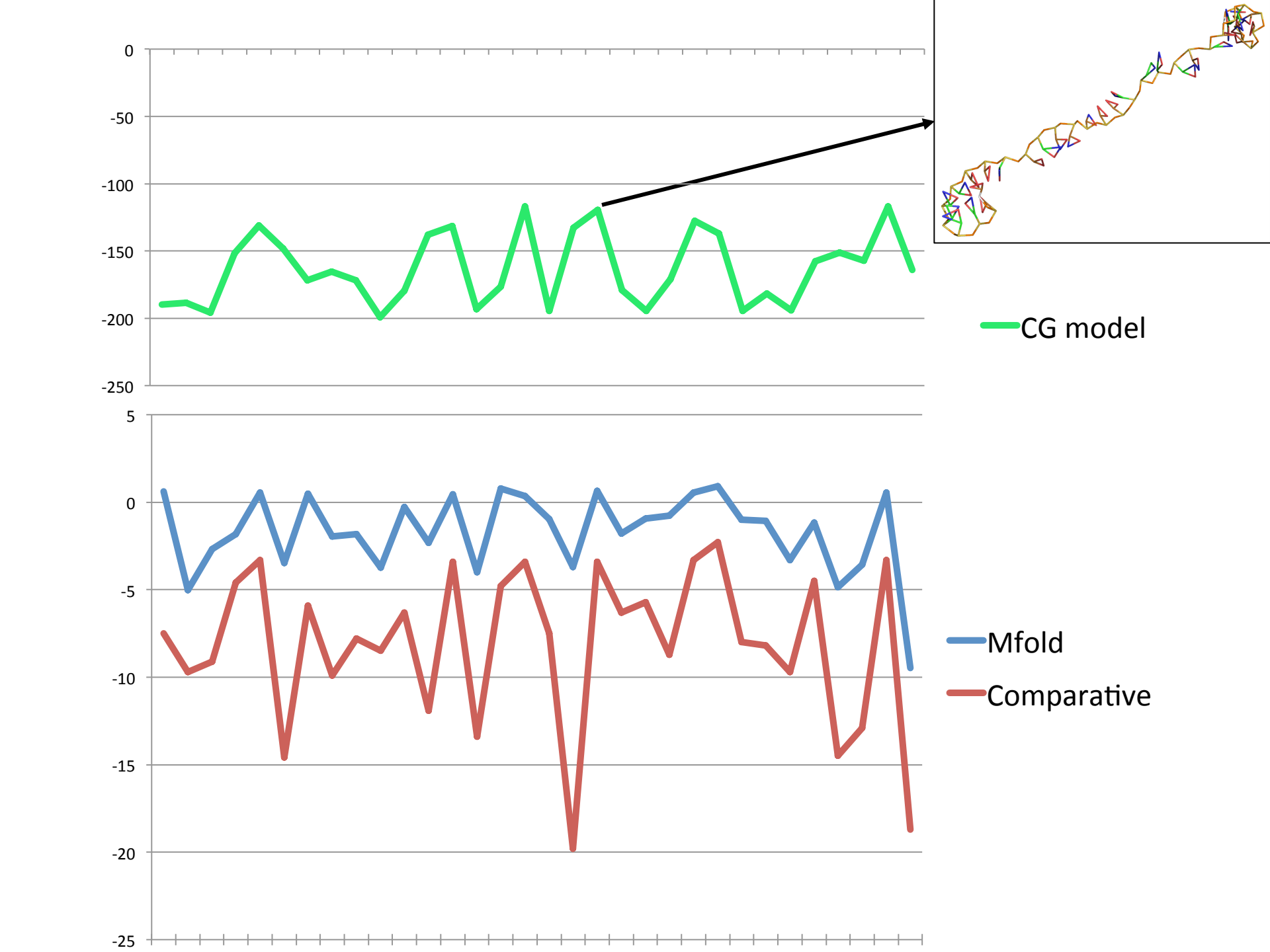
- Compile energies of last 100 snapshots
- Determine average and minimum energy values
- Compare cg model to Mfold[1]

[1] Zuker, M. (2003). "Mfold web server for nucleic acid folding and hybridization prediction." Nucleic Acids Research **31**(13): 3406-3415.

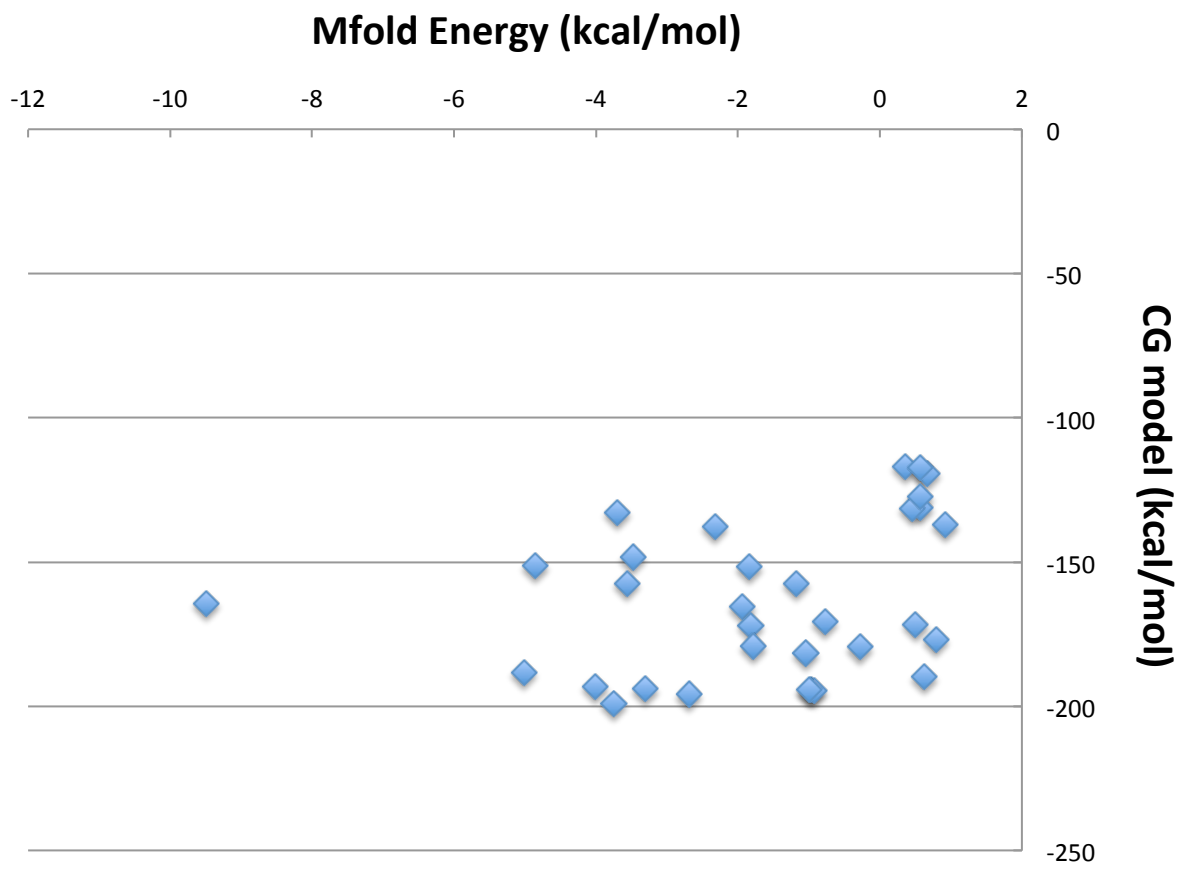
Mfold

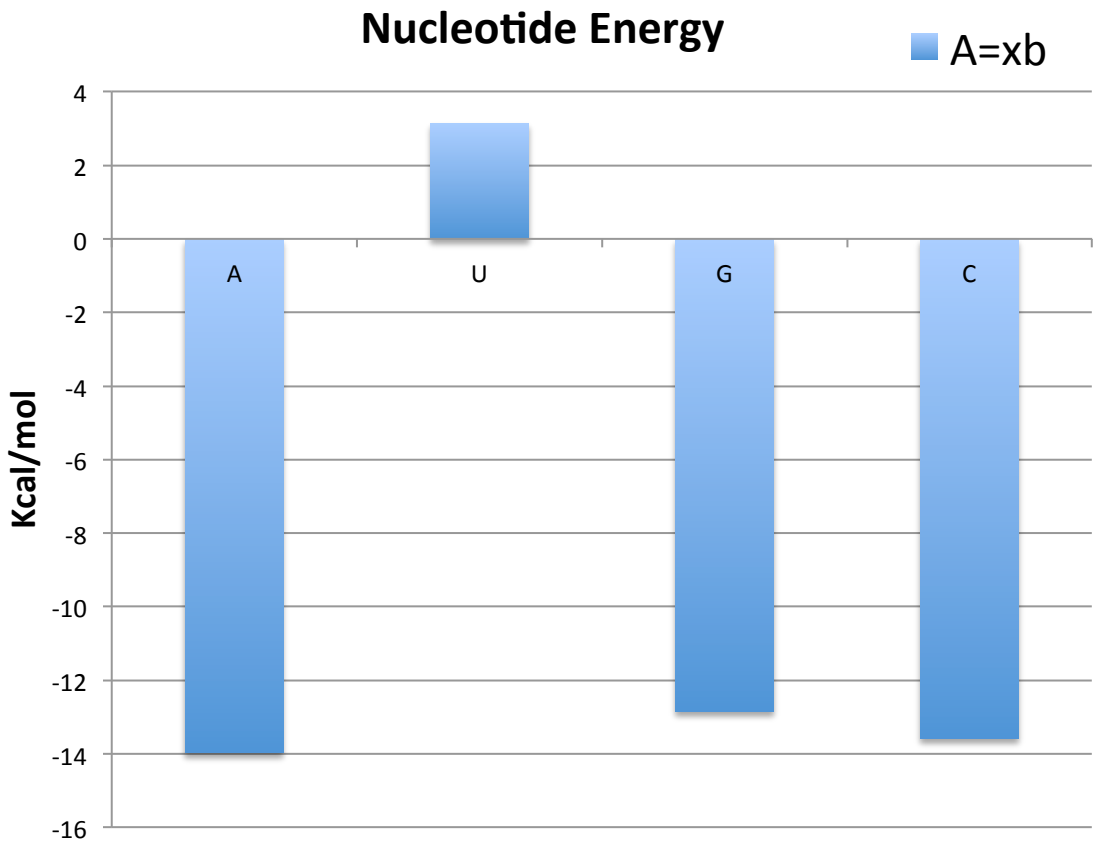
- Use web server
- Of 32 helices, 24 matched comparative

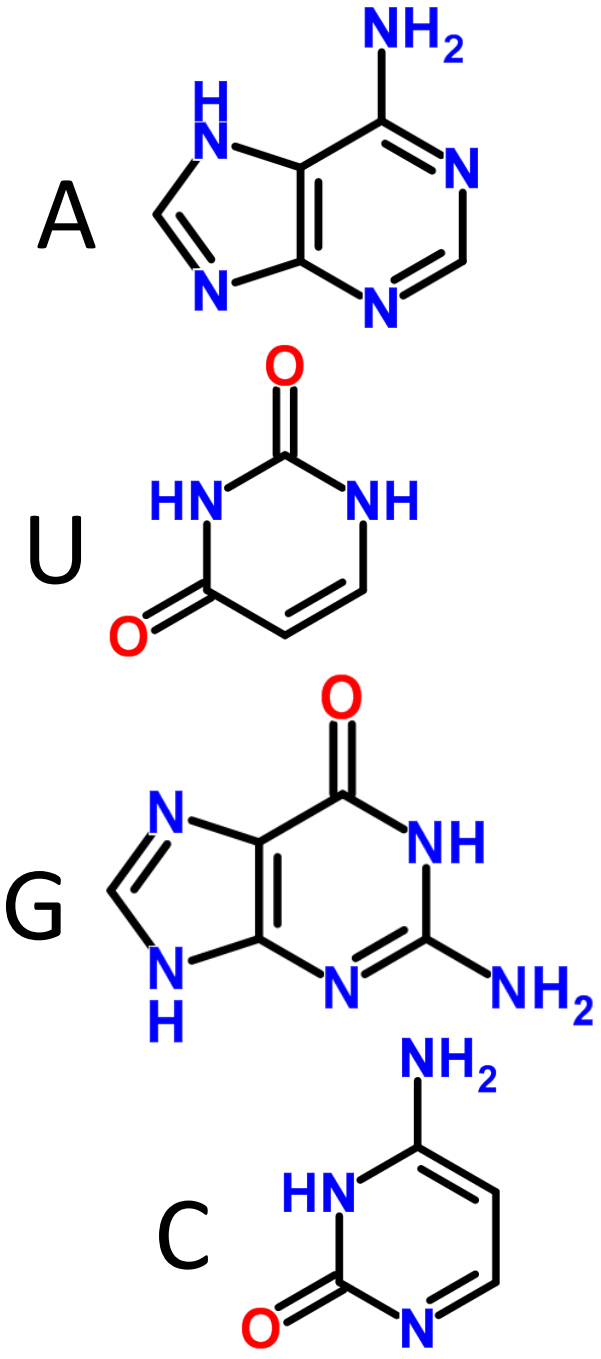
GAGUUUGAUCAUGGCUC;
GAAGAAGCUUGCUUCUUU;
CUACUGGAAACGGUAG;
GUCGCAAGAC;
CCUUCGGG;
UAGGUGGGGUAACGGCUCACCUA;
GUCUGAGAGGAU;
CUGGAACUGAGACACGGUCCAG;
CUCCUACGGGAG;
UGGGCGCAAGCCUG;
GGCCUUCGGGUU;
GAGUAAAGUUAAUACCUUUGCUC;
GCAGCCGC;
CCCGGGCUCAACCUGGG;
GCGGUGAAAUGC;
GCGAAGGC;


0
-50
-100
-150
-200
-250
CG model
5
0
-5
-10
-15
-20
-25
Mfold
Comparative

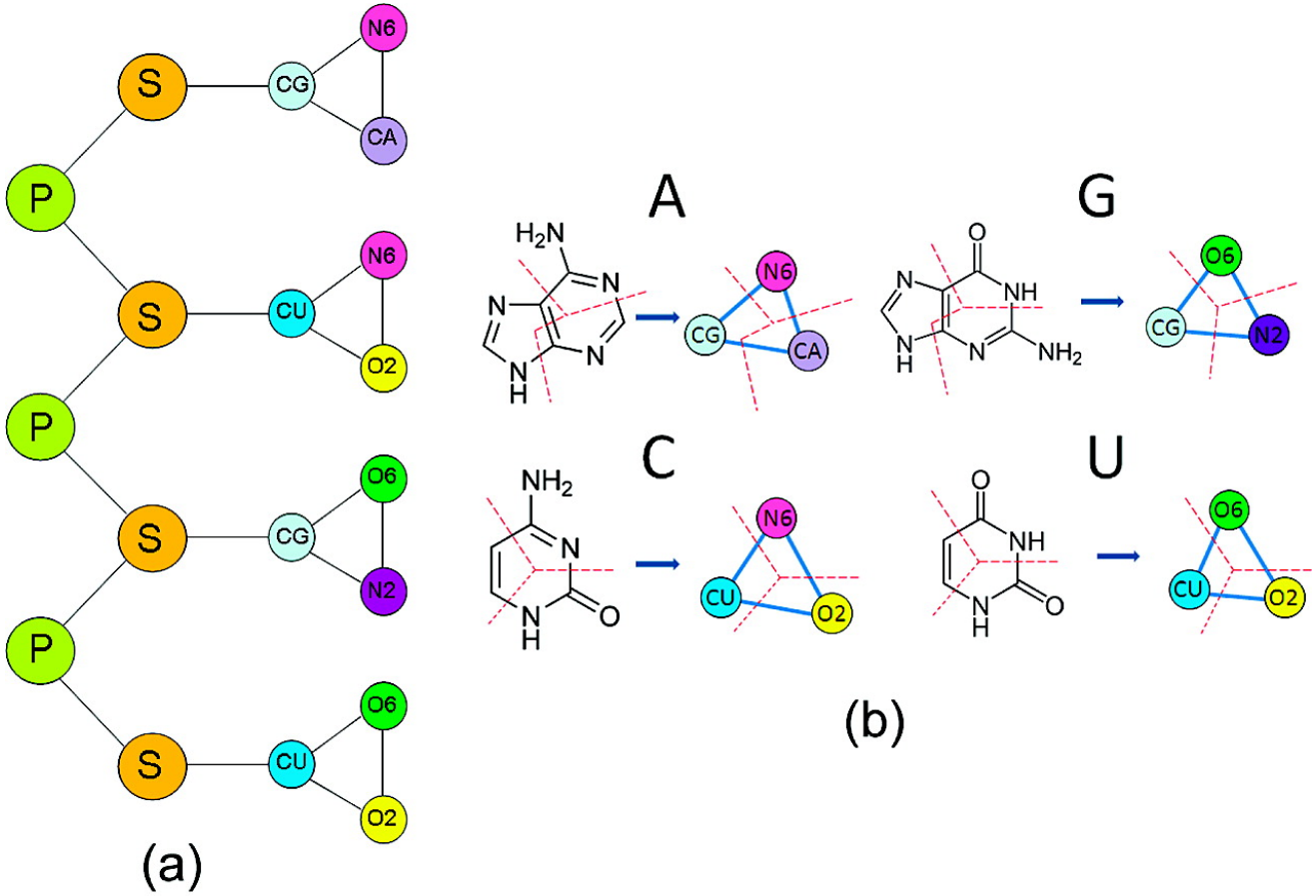
Correlation of Minimized Structures







*Structures from Chemspider



Ax=**b**

- The matrix A is not a basis (rank deficient,singular)

Improvements

- Current simulations
  - Longer simulation times for longer monlecules
  - Add base-pairing constraints
- Future simulations
  - Helix-only CG
  - Helix-only Mfold

